APPENDIX A

KowWin (LogKow) Log P Calculation:

SMILES : CN1(CCC24(C3(Oc5(c(O)ccc(CC1C2C= CC30)c45))))
CHEM :
MOL FOR: C17 H19 N1 O3
MOL WT : 285.35

TYPE	NUM	LOGKOW v1.66 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	0.5473	0.5473
Frag	3	-CH2- [aliphatic carbon]	0. 4911	1.4733
Frag	4	-CH [aliphatic carbon]	0.3614	1.4456
Frag	2	=CH - or =C< [olefinc carbon]	0 .3836	0.7672
Frag	1	-OH [hydroxy, aliphatic attach]	-1.4086	-1.4086
Frag	1	-N< [aliphatic attach]	-1.8323	-1.8323
Frag	6	Aromatic Carbon	0.2940	1.7640
Frag	1	-OH [hydroxy, aromatic attach]	-0.4802	-0.4802
Frag	1	-O- [oxygen, one aromatic attach]	-0.4664	-0.4664
Frag	1	-tert Carbon [3 or more carbon attach]	0.2676	0.2676
Factor	4	Fused aliphatic ring unit correction	-0.3421	-1.3684
Factor	1	Benzene to -C-C-N- correction	-0.2226	-0.2226
Const		Equation Constant		0.2290
			Log Kow =	0.7155

LogKow Estimated Log P: 0.72

Experimental Database Structure Match:
Name: Morphine
CAS Registry Number : 000057-27-2
Experimental Log Kow: 0.89
Experim. Reference : Avdeef,A et al. (1 996)

$$\frac{[n\text{-Butanol}]}{[\text{water}]} = \frac{5.25}{1}$$

KowWin (LogKow) Log P Calculation:

SMILES : Oc4(c1(c3(C(Cc2(ccc(OC)c(O)c12)) N(C)(C)CCc3cc4OC)))
CHEM :
MOL FOR: C20 H24 N1 O4 Magnoflorine
MOL WT : 342.42

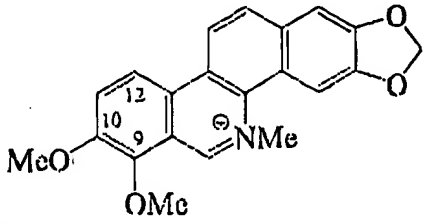
TYPE	NUM	LOGKOW v1.66 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	4	-CH3 [aliphatic carbon]	0.5473	2.1892
Frag	3	-CH2- [aliphatic carbon]	0. 4911	1.4733
Frag	1	-CH [aliphatic carbon]	0.3614	0.3614
Frag	12	Aromatic Carbon	0.2940	3.5280
Frag	2	-OH [hydroxy, aromatic attach]	-0.4802	-0.9604
Frag	2	-O- [oxygen, one aromatic attach]	-0.4664	-0.9328
Frag	1	>N< [+5 valence; single b onds;no H attach]	-6.6000	-6.6000
Factor	1	Fused aliphatic ring unit correction	-0.3421	-0.3421
Factor	2	Ring reaction -> alkyloxy ortho to -OH	-0.2560	-0.5120
Factor	1	Reaction: nitrogen[+5] / polar group	1.2500	1.2500
Const		Equation Constant		0.2290
			Log Kow =	-0.3164

LogKow Estimated Log P: -0.32

$$\frac{[n\text{-butanol}]}{[water]} = \frac{1}{2.1}$$

Entry Name: Chelerythrine

Synonym(s): 1,2-Dimethoxy-12-methyl[1,3]benzodioxolo[5,6-c]phenanthridinium(1+), sci. 7,8-Dimethoxy-10-methyl-2',3'-methylenedioxy-1,2-benzophenanthridinium(1+). Toddaline



Chapman & Hall Number: HGQ39-G
CAS Registry Number: 34316-15-9
Type of Compound Code(s): XA1950 VX3300 XA0650 XA1670 XA1700

Molecular Formula: $C_{21}H_{18}NO_4^{(+)}$
Molecular Weight: 348.377
Accurate Mass: 348.123584
Percentage Composition: C 72.40%; H 5.21%; N 4.02%; O 18.37%
General Statement: Several numbering systems have been used
Biological Source: Alkaloid from a wide variety of genera in the Papaveraceae (*Argemone, Bocconia, Chelidonium, Dicranostigma, Eschscholtzia, Glaucium, Hunnemannia, Hylomecon, Macleaya, Papaver, Platystemon, Sanguinaria, Stylomecon, Stylophorum*), Rutaceae (*Fagara, Toddalia, Zanthoxylum*), Fumariaceae (*Corydalis, Dicentra*), Sapindaceae (*Pteridophyllum*) and Hypecoaceae (*Hypecoum*)
Biological Use/Importance: Potent cytotoxic agent functioning by DNA intercalation and uncoupling of oxidative phosphorylation. Inhibitor of rat liver aminotransferases. Antimicrobial and antiinflammatory agent recommended for use against oral infections. Temporary hypertensive agent in mice, rabbits and cats. Analgesic. Antineoplastic agent. Prolongs sleep
Calculated Log P Data: Log P 0.11 (uncertain value) (calc)
UV: [neutral] λ_{max} 227 (); 282 (); 319 () (MeOH) (Berdy)

Derivative: Chloride
Chapman & Hall Number: HGP55-D
CAS Registry Number: 3895-92-9
Molecular Formula: $C_{21}H_{18}ClNO_4$
Molecular Weight: 383.83
Accurate Mass: 383.092436
Percentage Composition: C 65.71%; H 4.73%; Cl 9.24%; N 3.65%; O 16.67%
Physical Description: Cryst. + $1H_2O$ (dil. HCl)
Melting Point: Mp 213-214 dec. (193°, 202-203°, 207°)
Sigma: C2932